이학박사 학위논문

A Study on Efficient Algorithms for some Numerical Optimization Problems

수치 최적화 문제에 관한 효율적인 알고리즘에 대한 연구

2013 년 2 월

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Abstract

A Study on Efficient Algorithms for some Numerical Optimization Problems

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This thesis is mainly divided into two parts: parameter estimation problem in linear differential equations and a minimization algorithm which is applicable to some industrial problem.

In general, mathematical optimization problems are to find optimal elements of a set which minimize (or maximize) the value of a given objective function. It is well known problem and arises in a various field of applications such as science, engineering, business and so on. It has a long history and there are still very much a work in progress.

Optimization problems usually depend on the properties of objective functions involved. If functions are simple, *e.g.,* linear, the the problem is easy to solve and moreover mathematical theories completed. If it is complex, however, it is hard to solve it theoretically and/or numerically.

In this thesis, we suggest algorithms which is related to two specific optimization problems. These problems are both include nonlinear objective functions. The first part is to find a optimal parameter function of a differential equation and the second part is to find optimal solution of a facility location problem. Each parts contains theories about the solution, such as the existence and the uniqueness of the optimal solution, and numerical examples are included.

Keywords : Minimax problem, Numerical optimization, Facility location
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Part I

Parameter Estimation Problem

Chapter 1

Introduction

1.1 Background

Mathematical modeling using a system of differential equations with a set of parameters has been widely used in most scientific fields, such as, physics, chemistry, biology, earth and environmental sciences, and engineering. Mathematical problems related with such parameter-dependent differential equations can be categorized into forward and inverse problems. Forward problems need analysis and simulations of the model for given parameter values, while inverse problems require parameter estimation based on the measurements of output variables. The latter have drawn intensive attention for about three decades. For instance, see [5, 16], and the references therein. As statistical approaches to parameter estimation problems, nonlinear regression and other data fitting methods have been widely used [3, 4, 11, 12, 15].

Among various important problems related with parameter estimation, we are particularly interested in the problem of fitting parameter functions to given data by using a finite number of piecewise functions. The primary aim of this part is to propose and analyze efficient algorithms to estimate parameter functions. The number of subintervals and basis function in each subinterval are not known a priori, and then our main concerns are how to determine the number of subintervals and how to find time nodes for each subintervals optimally.

For a given data set, we are interested in finding a piecewise constant parameter function in a differential equation. A necessary and sufficient condition for existence and uniqueness of the piecewise constant parameter function in the case where the subintervals are known will be first sought. We also propose several criteria for determining the time nodes and then the parameter function in the case where the subintervals are yet to be determined. These criteria are provided by a C-test function in what follows. An algorithm is suggested to determine time nodes and coefficients for each subinterval optimally with the given data set and the number of subintervals. Several numerical experiments demonstrate that the algorithm is effective to estimate the parameter function. We also see that the solution of the linear differential equation with the estimated parameter function provides a good approximation for the solution of nonlinear differential equation.

1.2 Motivation

Numerous biological phenomena can be described by stage-structured modeling. For instance, the growth rates of most fishes are sensitive to seasonal effects, mainly to the temperature changes, and it has been well-known that there is a strong relationship between specific growth rate and temperature for the population of most bacteria. See, for instance, [6, 7, 17], and the references therein. Also, many delay differential equations with stage-structure can be found in the literature [1, 2, 9, 10, 13], and so on.

For a given data set $\{(p_j, q_j)\}_{j=1}^{J}, p_1 < p_2 < \cdots < p_J$, we consider the following stage-structured differential equation:

$$\frac{du}{dt} = f(t, u; \theta(t)), \quad t \in (p_1, p_J);$$
$$u(p_j) = q_j, \quad j = 1, \cdots, J.$$

with a parameter function

$$\theta(t) = \sum_{i=1}^{I} \theta_i \chi_{[t_{i-1}, t_i)}(t), \tag{1.1}$$

where the number of intervals I, the nodes t_i, and the parameters θ_i, $(i = 1, \cdots, I)$ are to be determined, assuming that $t_0 = p_1$. The parameters I, t_i, and θ_i depend on the differential equation and the given data set $\{(p_j, q_j)\}_{j=1}^{J}$.

1.3 Model problem

In this part, we will concentrate on linear differential equations with an emphasis on the relation between the parameter function and the data set. We now consider the following problem: for a set of given data $\{(p_j, q_j)\}_{j=1}^{J}$, find $\theta(t)$ in the form of (1.1) such that

$$\frac{du}{dt} = \theta(t)u, \quad t \in (p_1, p_J), \tag{1.2a}$$
$$u(p_j) = q_j \quad j = 1, \cdots, J. \tag{1.2b}$$

If $\theta(t)$ is known, the solution $u(t)$ of (1.2) is given by

$$u(t) = \sum_{i=1}^{I} u(t_{i-1}) e^{\theta_i (t - t_{i-1})} \chi_{[t_{i-1}, t_i)}(t). \tag{1.3}$$

Since most physical data are of positive values, we will assume that the solutions of Equation (1.2a) are positive and the data sets are restricted to such a case as described in Definition (1.3.1).

Definition 1.3.1. *A data set $D = \{(p_j, q_j)\}_{j=1}^J$ is called positively well-posed if D has the following two properties:*

1. *$\{p_j\}_{j=1}^J$ is a strictly increasing sequence;*
2. *$q_j > 0, \quad j = 1, \cdots, J.$*

If the number of subinterval is one, a necessary and sufficient condition for a constant function θ to be uniquely determined in the interval is summarized in the following lemma.

Lemma 1.3.2. *Suppose that there is a positively well-posed given data set $\{(p_j, q_j)\}_{j=1}^J$ in one interval $[t_0, t_1]$. Then one can uniquely determine the constant function θ and the solution $u(t)$ satisfying* (1.2) *if and only if*

$$\dim(\mathit{span}\{\, (1, p_j, \log q_j) \mid j = 1, \cdots, J \,\}) = 2.$$

The proof is easy, but we will give the details that will be useful in our further development.

Proof. Suppose that $u(t)$ satisfies that

$$u(t) = u(t_0)e^{\theta(t-t_0)},$$
$$u(p_j) = q_j, \quad j = 1, \cdots, J.$$

Then the given data set $\{(p_j, q_j)\}_{j=1}^J$ must satisfy

$$\log q_j = \log u(t_0) + \theta(p_j - t_0),$$

i.e., $\{(p_j, \log q_j)\}_{j=1}^J$ are collinear. The existence and uniqueness of $u(t_0)$ and θ are equivalent to

$$\dim(\text{span}\{(1, p_j, \log q_j) \mid j = 1, \cdots, J\}) = 2.$$

$\square$

Before describing the relation of data set, let us define a C-test function.

Definition 1.3.3. *Define a C-test function $C : (\mathbb{R} \times \mathbb{R}_+)^3 \to \mathbb{R}$ by*

$$C(x_1, y_1, x_2, y_2, x_3, y_3) := (x_1 - x_2) \log y_3 + (x_2 - x_3) \log y_1 + (x_3 - x_1) \log y_2.$$

Proposition 1.3.4. *Suppose that $x_1 < x_2 < x_3$. If $C(x_1, y_1, x_2, y_2, x_3, y_3)$ is positive(or negative), then there exists a log-concave (or log-convex) function which passes through (x_1, y_1), (x_2, y_2) and (x_3, y_3). Moreover the following properties hold:*

$$\begin{aligned} &C(x_1, y_1, x_2, y_2, x_3, y_3) = -C(x_1, y_1, x_3, y_3, x_2, y_2) \\ =\ &C(x_2, y_2, x_3, y_3, x_1, y_1) = -C(x_2, y_2, x_1, y_1, x_3, y_3) \\ =\ &C(x_3, y_3, x_1, y_1, x_2, y_2) = -C(x_3, y_3, x_2, y_2, x_1, y_1). \end{aligned} \tag{1.4}$$

Proof. Notice that $C(x_1, y_1, x_2, y_2, x_3, y_3)$ can be rewritten as

$$C(x_1, y_1, x_2, y_2, x_3, y_3) = (x_1 - x_2)(x_2 - x_3)\left[\frac{\log y_1 - \log y_2}{x_1 - x_2} - \frac{\log y_2 - \log y_3}{x_2 - x_3}\right].$$

Suppose that $C(x_1, y_1, x_2, y_2, x_3, y_3) > 0$. Then $(\log y_1 - \log y_2)/(x_1 - x_2) > (\log y_2 - \log y_3)/(x_2 - x_3)$ which implies that there exists a concave quadratic function which passes through $(x_1, \log y_1)$, $(x_2, \log y_2)$ and $(x_3, \log y_3)$. The case $C(x_1, y_1, x_2, y_2, x_3, y_3) < 0$ is similar. Equation (1.4) follows immediately from the definition of the C-test function C. $\square$

Remark 1.3.5. *$C(x_1, y_1, x_2, y_2, x_3, y_3) = 0$ implies that $(x_1, y_1), (x_2, y_2)$ and (x_3, y_3) lie on one exponential curve: $y = ae^{\theta x}$, where*

$$a = y_j \left(\frac{y_j}{y_k}\right)^{\frac{x_j}{x_k - x_j}}, \ \theta = \frac{\log y_k - \log y_j}{x_k - x_j} \quad \text{for } j, k = 1, 2, 3 \text{ such that } j \neq k.$$

Equivalently, the exponential curve can be rewritten by

$$y = y_j \left(\frac{y_k}{y_j}\right)^{\frac{x - x_j}{x_k - x_j}} \qquad \text{for } j, k = 1, 2, 3 \text{ such that } j \neq k.$$

Definition 1.3.6. *A data set $D = \{(p_j, q_j)\}_{j=1}^J$ is called reducible for a parameter estimation problem if and only if there exist three adjacent data points $\{(p_j, q_j), (p_{j+1}, q_{j+1}), (p_{j+2}, q_{j+2})\}$, such that $C(p_j, q_j, p_{j+1}, q_{j+1}, p_{j+2}, q_{j+2}) = 0$ for any $j \in \{1, \cdots, J-2\}$. Otherwise, the set of data $D = \{(p_j, q_j)\}_{j=1}^J$ is called irreducible for a parameter estimation problem.*

Remark 1.3.7. *If a given data set $\{(p_j, q_j)\}_{j=1}^J$ is positively well-posed and irreducible in an interval $[t_0, t_I]$ with a partition $\cup_{i=1}^I [t_{i-1}, t_i)$, then every subinterval contains no more than two data points if the data set determines the parameter function $\theta(t)$ uniquely fulfilling* (1.2).

Chapter 2

Basic Properties of Algorithm

2.1 Case Study

2.1.1 The case where the subintervals are known

We begin by looking at the case where t_i, $(i = 1, \cdots, I)$, are given. The following theorem gives the conditions for the given data set to guarantee the existence and uniqueness of the parameter function $\theta(t)$ and the corresponding solution $u(t)$ of (1.2).

Theorem 2.1.1. *Let $I = J - 1$. Suppose that a given data set $\{(p_j, q_j)\}_{j=1}^{J}$ is positively well-posed and let $t_0 < t_1 < \cdots < t_I$ be given time nodes of $[t_0, t_I]$. Then there exist a unique parameter function $\theta(t)$ and its solution $u(t)$ which satisfy* (1.2) *if and only if the following condition holds:*

If any interval $[t_{k-1}, t_k)$ contains two data points, $k - 1$ data points are located in $[t_0, t_{k-1})$, $(k = 1, \cdots, I)$.

Proof. Let us rearrange the data points as follows:

i) For $1 \le i \le I$, let m_i be the number of data points in the interval $[t_{i-1}, t_i)$ so that $m_1 + \cdots + m_I = J$ and $m_i \in \{0, 1, 2\}$;

ii) For $1 \le i \le I$, denote $\{(p^i_j, q^i_j)\}_{j=1}^{m_i}$ by the set of data points in the interval $[t_{i-1}, t_i)$;

iii) For $1 \le i \le I$, $\{p^i_j\}_{j=1}^{m_i}$ is a strictly increasing sequence.

Suppose that there is a continuous function $u(t)$ which satisfies

$$\begin{cases} u(t) = \displaystyle\sum_{i=1}^{I} \left[u(t_{i-1}) e^{\theta_i (t - t_{i-1})} \right] \chi_{[t_{i-1}, t_i)}(t). \\ u(p^i_j) = q^i_j, \quad j = 1, \cdots, m_i, \quad i = 1, \cdots, I. \end{cases}$$

Then the given data (p^i_j, q^i_j) must satisfy

$$\log q^i_j = \log u(t_{i-1}) + \theta_i (p^i_j - t_{i-1}) \quad \text{for } 1 \le j \le m_i \text{ and } 1 \le i \le I. \tag{2.1}$$

And by the continuity conditions, we obtain

$$\log u(t_i) = \log u(t_{i-1}) + \theta_i (t_i - t_{i-1}) \quad \text{for } 1 \le i \le I - 1. \tag{2.2}$$

Set

$$\begin{aligned} \boldsymbol{x} &= (\log u(t_0), \theta_1, \log u(t_1), \theta_2, \cdots, \log u(t_{I-1}), \theta_I)^t \in \mathbb{R}^{2I}, \\ \boldsymbol{b} &= \left(\log q^1_1, \cdots, \log q^1_{m_1}, 0, \log q^2_1, \cdots, \log q^2_{m_2}, 0, \cdots, 0, \log q^I_1, \cdots, \log q^I_{m_I}\right)^t \\ &\quad \in \mathbb{R}^{J+I-1}. \end{aligned}$$

Combining (2.1) and (2.2), we have

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b},$$

where the $(J+I-1)\times 2I$ matrix $\boldsymbol{A}$ is explicitly given by

$$\boldsymbol{A} = \begin{bmatrix}
1 & (p_1^1 - t_0) & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\
1 & (p_{m_1}^1 - t_0) & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\
1 & (t_1 - t_0) & -1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & (p_1^2 - t_1) & 0 & \cdots & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 1 & (p_{m_2}^2 - t_1) & 0 & \cdots & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & (t_2 - t_1) & -1 & \cdots & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & \cdots & 1 & (p^{I-1} - t_{I-1}) & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & \cdots & 1 & (p^{I-1} - t_{I-1}) & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \cdots & 1 & (t_I - t_{I-1}) & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & (p_1^I - t_{I-1}) \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 1 & (p_{m_I}^I - t_{I-1})
\end{bmatrix}.$$

It then follows that the existence of a unique parameter function $\theta(t)$ and the corresponding function $u(t)$ which satisfy (1.2) is equivalent to the invertibility of the matrix $\boldsymbol{A}$. Since $m_i \leq 2$ $(i = 1, \cdots, I)$ and $I = J-1$, there exists at least one $k \in \{1, \cdots, I\}$ such that $m_k = 2$ by the pigeon hole principle.

With the help of elementary operations, $\boldsymbol{A}$ can be transformed into a matrix

$$\boldsymbol{A} \sim \begin{bmatrix} \mathbf{A_1} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{A_2} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{A_3} \end{bmatrix},$$

where $\mathbf{0}$ denoting a zero block matrix and

$$\mathbf{A_1} = \begin{bmatrix} 1 & (p_1^1 - t_0) & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & (p_{m_1}^1 - t_0) & 0 & \cdots & 0 & 0 \\ 1 & (t_1 - t_0) & -1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & (p_1^{k-1} - t_{k-2}) \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & (p_{m_{k-1}}^{k-1} - t_{k-2}) \\ 0 & 0 & 0 & \cdots & 1 & (t_{k-1} - t_{k-2}) \end{bmatrix}$$

$$\mathbf{A_2} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$\mathbf{A_3} = \begin{bmatrix} -1 & 0 & 0 & \cdots & 0 & 0 \\ 1 & (p_1^{k+1} - t_k) & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & (p_{m_{k+1}}^{k+1} - t_k) & 0 & \cdots & 0 & 0 \\ 1 & (t_{k+1} - t_k) & -1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & (p_1^I - t_{I-1}) \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & (p_{m_I}^I - t_{I-1}) \end{bmatrix}.$$

Since

$$
\begin{aligned}
&\operatorname{rank}(\mathbf{A_1}) \leq \min\{\, m_1 + \cdots + m_{k-1} + (k-1),\, 2(k-1)\,\},\\
&\operatorname{rank}(\mathbf{A_2}) = 2,\\
&\operatorname{rank}(\mathbf{A_3}) \leq \min\{\, m_{k+1} + \cdots + m_I + (I-k),\, 2(I-k)\,\},
\end{aligned}
$$

recalling $I = J + 1 = \sum_{j=1}^{I} m_j + 1$, we obtain

$$
\begin{aligned}
\operatorname{rank}(\boldsymbol{A}) = {} & \operatorname{rank}(\mathbf{A_1}) + \operatorname{rank}(\mathbf{A_2}) + \operatorname{rank}(\mathbf{A_3})\\
\leq {} & \min\{\, m_1 + \cdots + m_{k-1} + (k-1),\, 2(k-1)\,\} + 2\\
& + \min\{\, m_{k+1} + \cdots + m_I + (I-k),\, 2(I-k)\,\}\\
= {} & \min\{\, m_1 + \cdots + m_{k-1} + (k-1),\, 2(k-1)\,\} + 2\\
& \min\{\, (2I-k-1) - (m_1 + \cdots + m_{k-1}),\, 2(I-k)\,\}\\
= {} & \min\{\, m_1 + \cdots + m_{k-1},\, k-1\,\} + (k-1) + 2\\
& - \max\{\, m_1 + \cdots + m_{k-1},\, k-1\,\} + (2I-k-1).
\end{aligned}
$$

Hence in the case of $m_1 + \cdots + m_{k-1} \neq k-1$, $\operatorname{rank}(\boldsymbol{A}) < 2I$ and thus $\boldsymbol{A}$ is not invertible. Thus we need a condition $m_1 + \cdots + m_{k-1} = k-1$ with $m_k = 2$ to make that $\boldsymbol{A}$ is invertible. □

Remark 2.1.2. *i) Theorem 2.1.1 gives the necessary and sufficient condition for data and subintervals in order to determine a parameter function $\theta(t)$ uniquely which fulfills* (1.2)*. That is, if a subinterval contains two data points, then the number of data points should equal to the number of subintervals in the whole left side of the interval.*

ii) In the case of $I > J-1$, we have rank($\boldsymbol{A}$) $\leq J+I-1 < 2I$, and hence $\mathbf{A}$ is not invertible. Although one may determine $\theta(t)$, one does not guarantee the uniqueness of the parameter function $\theta(t)$ and the corresponding *function* $u(t)$ *which satisfy* (1.2).

iii) *In the case of* $I < J - 1$, *we have an over-determined problem. The only case where the over-determined system* $\boldsymbol{A}\boldsymbol{x} = \mathbf{b}$ *has a unique solution is that the linear system can be reduced to the system* $\mathbf{A}'\boldsymbol{x} = \mathbf{b}'$ *with rank*$(\mathbf{A}') = 2I$.

Example 2.1.3. *Let* $\{(p_j, q_j)\}_{j=1}^{J}$ *and* $t_0 < t_1 < \cdots < t_I$ *be a given positively well-posed data set and given time nodes in* $[t_0, t_I]$ *with* $I = J-1$. *Suppose that there happens to be two consecutive subintervals,* $[t_{k-1}, t_k)$ *and* $[t_k, t_{k+1})$ *that contain two data points in each subinterval, then the parameter function* $\theta(t)$ *cannot be determined uniquely. Indeed, in order for the parameter function* $\theta(t)$ *to be determined uniquely, by Theorem 2.1.1,* $[t_0, t_{k-1})$ *contains* $k - 1$ *data points and* $[t_0, t_k)$ *contains* k *data points, which leads to a contradiction.*

2.1.2 The case where the subintervals are yet to be determined

The previous section describes the necessary and sufficient conditions for a data set to determine a parameter function and its corresponding solution uniquely when $I = J - 1$. The parameter function estimation problem is over-determined in the case of $I < J - 1$. If the problem is over-determined with too much information then a particular solution may not exist. As one way to overcome this problem, we can increase the number of unknown parameters by considering the time nodes $\{t_i\}_{i=1}^{I-1}$ are also to be determined. Suppose the given data set $\{(p_j, q_j)\}_{j=1}^{J}$ is positively well-posed and irreducible. Then every subinterval should have at most two data points. Notice that in each subinterval the constant value of the parameter θ and its corresponding solution $u(t)$ is uniquely determined by two data points. Thus in order to determine the parameter function for whole interval, we need to consider the following types of contiguous subintervals.

T1. Each of the first and last subintervals in this category contains two data points while each of all the others contains one data point;

T2. Only one of the first and last subintervals in this category contains two data points while each of all the others contains one data point;

In the cases of T2, the existence of t_i and the corresponding parameters θ_i is always guaranteed. So, we focus our attention on the case of T1 in this section. Note that $I = J - 2$ in the case of T1.

Lemma 2.1.4. *Assume that x_1, x_2 and x_3 are any nonzero real numbers. Then the following are equivalent:*

i) $x_1 \cdot x_3 < 0$ *or* $x_2 \cdot x_3 > 0$;

ii) $x_1 \cdot x_2 > 0$ *or* $x_2 \cdot x_3 > 0$.

Proof. Suppose *ii)* is not true, i.e.,

$$x_1 \cdot x_2 < 0 \text{ and } x_2 \cdot x_3 < 0.$$

Then

$$x_1 \cdot x_3 > 0 \text{ and } x_2 \cdot x_3 > 0$$

and this implies that *i)* is not true. By contrapositive, this completes the proof. □

Proposition 2.1.5. *Suppose that $I = 2$ and the given data set $\{(p_j, q_j)\}_{j=1}^4$ is positively well-posed and irreducible over the whole interval $[t_0, t_2]$. Then there exist unique $t_1 \in [p_2, p_3]$ and the corresponding parameters θ_1, θ_2 such that the function $u(t)$ given by (1.3) satisfies (1.2) if and only if*

$$C(p_1, q_1, p_2, q_2, p_3, q_3) \times C(p_2, q_2, p_3, q_3, p_4, q_4) \geq 0.$$

Proof. Suppose that there exists $t_1 \in [p_2, p_3]$ and the corresponding parameters θ_1, θ_2 such that the function $u(t)$ given by (1.3) satisfies (1.2). Then we have

$$u(t) = u(t_0)e^{\theta_1(t-t_0)}\chi_{[t_0,t_1)}(t) + u(t_1)e^{\theta_2(t-t_1)}\chi_{[t_1,t_2)}(t) \in C^0(t_0, t_2)$$

and (1.2b) also requires further relations,

$$\begin{aligned} u(t_0)e^{\theta_1(p_1-t_0)} &= q_1, \quad u(t_0)e^{\theta_1(p_2-t_0)} = q_2, \\ u(t_1)e^{\theta_2(p_3-t_1)} &= q_3, \quad u(t_1)e^{\theta_2(p_4-t_1)} = q_4. \end{aligned}$$

By solving the above equations, the parameter values of θ_1 and θ_2 and the logarithmic values of $u(t_0)$ and $u(t_1)$ can be determined in terms of $\{(p_j, q_j)\}_{j=1}^4$;

$$\begin{aligned} \theta_1 &= \frac{\log q_1 - \log q_2}{p_1 - p_2}, \quad \theta_2 = \frac{\log q_3 - \log q_4}{p_3 - p_4}, \\ \log u(t_0) &= \frac{\log q_1 - \log q_2}{p_1 - p_2} t_0 + \frac{p_1 \log q_2 - p_2 \log q_1}{p_1 - p_2}, \\ \log u(t_1) &= \frac{\log q_3 - \log q_4}{p_3 - p_4} t_1 + \frac{p_3 \log q_4 - p_4 \log q_3}{p_3 - p_4}. \end{aligned} \tag{2.3}$$

From the continuity condition $\lim_{t \to t_1 -} u(t) = u(t_1)$, we have

$$u(t_1) = u(t_0)e^{\theta_1(t_1-t_0)}.$$

Substituting the values (2.3) gives

$$\frac{\log q_3 - \log q_4}{p_3 - p_4} t_1 + \frac{p_3 \log q_4 - p_4 \log q_3}{p_3 - p_4} = \frac{\log q_1 - \log q_2}{p_1 - p_2} t_1 + \frac{p_1 \log q_2 - p_2 \log q_1}{p_1 - p_2}, \tag{2.4}$$

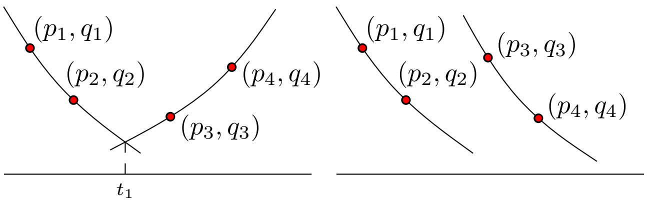
and we finally get

$$t_1 = -\left(\frac{p_1 \log q_2 - p_2 \log q_1}{p_1 - p_2} - \frac{p_3 \log q_4 - p_4 \log q_3}{p_3 - p_4}\right) \times \left(\frac{\log q_1 - \log q_2}{p_1 - p_2} - \frac{\log q_3 - \log q_4}{p_3 - p_4}\right)^{-1}.$$

Now we want to derive a condition in which t_1 lies within p_2 and p_3 (see Figure 2.1). The condition can be restated as $(t_1 - p_2)(t_1 - p_3) \leq 0$, and by direct calculation, we have

$$\begin{aligned} 0 &\geq (t_1 - p_2)(t_1 - p_3) \\ &= -\frac{C(p_1, q_1, p_2, q_2, p_3, q_3) \times C(p_2, q_2, p_3, q_3, p_4, q_4)}{(p_1 - p_2)(p_3 - p_4)\left(\frac{\log q_1 - \log q_2}{p_1 - p_2} - \frac{\log q_3 - \log q_4}{p_3 - p_4}\right)^2}. \end{aligned}$$

Note that the denominator is not zero since data points are irreducible. Thus we have $t_1 \in [p_2, p_3]$ if and only if $C(p_1, q_1, p_2, q_2, p_3, q_3) \times C(p_2, q_2, p_3, q_3, p_4, q_4) \geq 0$. $\square$



(a) C-test successes (b) C-test fails

Figure 2.1: For given data with $I = 2$, t_1 can be uniquely determined in the case (a) while t_1 cannot be determined in the case (b).

Lemma 2.1.6. *Suppose that $I = 3$ and the given data set $\{(p_j, q_j)\}_{j=1}^5$ is positively well-posed and irreducible over the whole interval $[t_0, t_3]$. Then there exist $t_1 \in [p_2, p_3]$, $t_2 \in [p_3, p_4]$ and corresponding parameters θ_1, θ_2 and θ_3 such* *that the function $u(t)$ given by* (1.3) *satisfies* (1.2) *if and only if*

$$
\begin{aligned}
& C(p_1,q_1,p_2,q_2,p_3,q_3) \times C(p_2,q_2,p_3,q_3,p_4,q_4) \geq 0; \\
\text{or} \quad & C(p_2,q_2,p_3,q_3,p_4,q_4) \times C(p_3,q_3,p_4,q_4,p_5,q_5) \geq 0
\end{aligned}
$$

Proof. Suppose that there exist two free nodes t_1 and t_2 such that following conditions hold (see Figure 2.2):

$$
\begin{aligned}
u(t_0)e^{\theta_1(p_1-t_0)} &= q_1, \quad & u(t_0)e^{\theta_1(p_2-t_0)} &= q_2, \\
u(t_1)e^{\theta_2(p_3-t_1)} &= q_3, \quad & u(t_2)e^{\theta_3(p_4-t_2)} &= q_4, \\
& & u(t_2)e^{\theta_3(p_5-t_2)} &= q_5.
\end{aligned} \tag{2.5}
$$

For this problem, we have to determine eight variables $\theta_1, \theta_2, \theta_3, u(t_0), u(t_1), u(t_2), t_1$, and t_2. From (2.5), it is clear that

$$
\begin{aligned}
\theta_1 &= \frac{\log q_1 - \log q_2}{p_1 - p_2}, \quad \theta_3 = \frac{\log q_4 - \log q_5}{p_4 - p_5}, \\
\log u(t_0) &= \frac{\log q_1 - \log q_2}{p_1 - p_2} t_0 + \frac{p_1 \log q_2 - p_2 \log q_1}{p_1 - p_2}, \\
\log u(t_2) &= \frac{\log q_4 - \log q_5}{p_4 - p_5} t_2 + \frac{p_4 \log q_5 - p_5 \log q_4}{p_4 - p_5}
\end{aligned} \tag{2.6}
$$

By the continuity condition of the solution, we obtain

$$
\begin{aligned}
\log u(t_1) &= \frac{\log q_1 - \log q_2}{p_1 - p_2} t_1 + \frac{p_1 \log q_2 - p_2 \log q_1}{p_1 - p_2}, \\
& u(t_1)e^{\theta_2(t_2-t_1)} = u(t_2).
\end{aligned} \tag{2.7}
$$

Thus $\theta_1, \theta_3, u(t_0), u(t_1)$ and $u(t_2)$ can be determined by t_1, t_2, θ_2 and data set $\{(p_j, q_j)\}_{j=1}^5$. However, θ_2 has a relation with t_1 and t_2. Thus showing the existence of θ_2 is equivalent to showing that the algebraic system

$$\log q_3 - \log u(t_1) = \theta_2(p_3 - t_1),$$
$$\log u(t_2) - \log u(t_1) = \theta_2(t_2 - t_1)$$

has at least one solution θ_2. This leads to the relation

$$\frac{\log q_3 - \log u(t_1)}{p_3 - t_1} = \frac{\log u(t_2) - \log u(t_1)}{t_2 - t_1},$$

which is equivalent to

$$(p_3 - t_2)\log u(t_1) - (t_1 - t_2)\log q_3 + (t_1 - p_3)\log u(t_2) = 0. \tag{2.8}$$

Combining equations (2.6), (2.7) and (2.8), one gets

$$\begin{aligned} 0 = &\left[\frac{\log q_1 - \log q_2}{p_1 - p_2} - \frac{\log q_4 - \log q_5}{p_4 - p_5}\right] t_1 t_2 \\ &- \left[\frac{\log q_1 - \log q_2}{p_1 - p_2} p_3 - \log q_3 + \frac{p_4 \log q_5 - p_5 \log q_4}{p_4 - p_5}\right] t_1 \\ &+ \left[\frac{p_1 \log q_2 - p_2 \log q_1}{p_1 - p_2} - \log q_3 + \frac{\log q_4 - \log q_5}{p_4 - p_5} p_3\right] t_2 \\ &- \left[\frac{p_1 \log q_2 - p_2 \log q_1}{p_1 - p_2} - \frac{p_4 \log q_5 - p_5 \log q_4}{p_4 - p_5}\right] p_3. \end{aligned} \tag{2.9}$$

We denote the RHS of (2.9) as $f(t_1, t_2)$. Now we consider the roots of the function f on the rectangular domain $[p_2, p_3] \times [p_3, p_4]$. Since f is a polynomial of t_1, t_2 and $f(p_3, p_3) = 0$, function $f(t_1, t_2)$ has roots on the domain $[p_2, p_3] \times [p_3, p_4]$, provided

$$f(p_2, p_3) \times f(p_2, p_4) \le 0 \quad \text{or} \quad f(p_2, p_4) \times f(p_3, p_4) \le 0.$$

Representing the above conditions using C-function (see Appendix), we obtain

$$
\begin{aligned}
& C(p_1, q_1, p_2, q_2, p_3, q_3) \times C(p_2, q_2, p_3, q_3, p_4, q_4) \geq 0 \\
\text{or} \quad & C(p_2, q_2, p_3, q_3, p_4, q_4) \times C(p_3, q_3, p_4, q_4, p_5, q_5) \geq 0
\end{aligned}
$$

which completes the proof. □

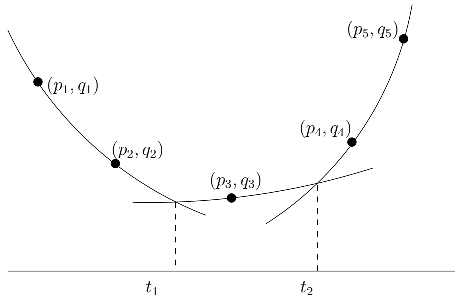


Figure 2.2: An example of the case where five data points satisfy the C-test condition.

Lemma 2.1.6 can be extended to general cases.

Theorem 2.1.7 (C-test)**.** *Suppose that* $I = n + 2$ *(* n *is positive integer) and the given data set* $\{(p_j, q_j)\}_{j=1}^{n+4}$ *is positively well-posed and irreducible over the whole interval* $[t_0, t_{n+2}]$*. Then there exist* $t_i \in [p_{i+1}, p_{i+2}]$ *for all* $i = 1, \cdots, n+1$*, and corresponding parameters* $\theta_1, \cdots, \theta_{n+2}$ *such that the function* $u(t)$ *given by* (1.3) *satisfies* (1.2) *if and only if*

$$C(p_i, q_i, p_{i+1}, q_{i+1}, p_{i+2}, q_{i+2}) \times C(p_{i+1}, q_{i+1}, p_{i+2}, q_{i+2}, p_{i+3}, q_{i+3}) \geq 0, \quad (2.10)$$

for some $i \in \{1, \cdots, n+1\}$.

Proof. As in Lemma 2.1.6, the theorem is correct for $n = 1$. Assume it is true for $n - 1$.

($\Rightarrow$) Suppose that there exist $t_i \in [p_{i+1}, p_{i+2}]$ for all $i = 1, \cdots, n+1$, and corresponding parameters $\theta_1, \cdots, \theta_{n+2}$ such that the function $u(t)$ given by (1.3) satisfies (1.2). By the continuity condition as in the equation (2.4), we have

$$\log u(t_1) = \frac{\log q_1 - \log q_2}{p_1 - p_2} t_1 + \frac{p_1 \log q_2 - p_2 \log q_1}{p_1 - p_2}.$$

Now we consider a new data set $\{(t_1, u(t_1))\} \cup \{(p_j, q_j)\}_{j=3}^{n+4}$. Since the theorem holds for $n-1$, it is true that

$$\begin{aligned} & C(t_1, u(t_1), p_3, q_3, p_4, q_4) \times C(p_3, q_3, p_4, q_4, p_5, q_5) \geq 0 \\ \text{or} \quad & C(p_i, q_i, p_{i+1}, q_{i+1}, p_{i+2}, q_{i+2}) \times C(p_{i+1}, q_{i+1}, p_{i+2}, q_{i+2}, p_{i+3}, q_{i+3}) \geq 0 \end{aligned} \tag{2.11}$$

for some $i \in \{3, \cdots, n+1\}$.

Define $L : \mathbb{R} \to \mathbb{R}$ by $L(t_1) := C(t_1, u(t_1), p_3, q_3, p_4, q_4)$, that is,

$$\begin{aligned} L(t_1) &= (p_3 - p_4) \log u(t_1) + (p_4 - t_1) \log q_3 + (t_1 - p_3) \log q_4 \\ &= (p_3 - p_4) \left(\frac{\log q_1 - \log q_2}{p_1 - p_2} t_1 + \frac{p_1 \log q_2 - p_2 \log q_1}{p_1 - p_2} \right) \\ &\quad + (p_4 - t_1) \log q_3 + (t_1 - p_3) \log q_4. \end{aligned}$$

Since L is a linear function of t_1 and $p_2 \leq t_1 \leq p_3$, the condition (2.11) implies

$$L(p_2) \times C(p_3, q_3, p_4, q_4, p_5, q_5) \geq 0 \quad \text{or} \quad L(p_3) \times C(p_3, q_3, p_4, q_4, p_5, q_5) \geq 0.$$

From the calculation, we get

$$\begin{aligned} & L(p_2) \times C(p_3, q_3, p_4, q_4, p_5, q_5) \\ & = C(p_2, q_2, p_3, q_3, p_4, q_4) \times C(p_3, q_3, p_4, q_4, p_5, q_5), \end{aligned}$$

and

$$
\begin{aligned}
&L(p_3) \times C(p_3, q_3, p_4, q_4, p_5, q_5) \\
&= -\left(\frac{p_3 - p_4}{p_1 - p_2}\right) \times C(p_1, q_1, p_2, q_2, p_3, q_3) \times C(p_3, q_3, p_4, q_4, p_5, q_5).
\end{aligned}
$$

Therefore we have

$$
\begin{aligned}
&C(p_2, q_2, p_3, q_3, p_4, q_4) \times C(p_3, q_3, p_4, q_4, p_5, q_5) \geq 0 \\
\text{or} \quad &C(p_1, q_1, p_2, q_2, p_3, q_3) \times C(p_3, q_3, p_4, q_4, p_5, q_5) \leq 0.
\end{aligned}
$$

By Lemma 2.1.4, we obtain

$$
\begin{aligned}
&C(p_1, q_1, p_2, q_2, p_3, q_3) \times C(p_2, q_2, p_3, q_3, p_4, q_4) \geq 0 \\
\text{or} \quad &C(p_2, q_2, p_3, q_3, p_4, q_4) \times C(p_3, q_3, p_4, q_4, p_5, q_5) \geq 0.
\end{aligned}
$$

This means that there exists $i \in \{1, \cdots, n+1\}$ such that (2.10) holds.

($\Leftarrow$) Suppose that (2.10) holds for some $i \in \{1, \cdots, n\}$. Then we consider a new data set $\{(p_j, q_j)\}_{j=1}^{n+3}$. Since the theorem holds for $n-1$, it is true that there exist $t_i \in [p_{i+1}, p_{i+2}]$ for all $i = 1, \cdots, n$, and corresponding parameters $\theta_1, \cdots, \theta_{n+1}$ such that the function $u(t)$ given by (1.3) satisfies (1.2). If we choose $t_{n+1} = p_{n+3}$, then we can determine θ_{n+2} such that the function $u(t)$ on the subinterval $[t_{n+1}, t_{n+2}]$ is passing the data point (p_{n+4}, q_{n+4}).

Suppose that (2.10) is true for some $i = n+1$. Then we consider a new data set $\{(p_j, q_j)\}_{j=2}^{n+4}$. By similar arguments, we can construct $t_i \in [p_{i+1}, p_{i+2}]$ for all $i = 1, \cdots, n+1$, and corresponding parameters $\theta_1, \cdots, \theta_{n+2}$. $\square$

Remark 2.1.8. *Under the assumption on irreducibility of data points, the value of C-function is always nonzero. From this fact, we can rewrite the condition* (2.10) *as* (2.12).

Theorem 2.1.9 (modified C-test)**.** *Suppose that $I = n + 2$ (n is positive integer) and the given data set $\{(p_j, q_j)\}_{j=1}^{n+4}$ is positively well-posed and irreducible over the whole interval $[t_0, t_{n+2}]$. Then there exist $t_i \in [p_{i+1}, p_{i+2}]$ for all $i = 1, \cdots, n+1$, and corresponding parameters $\theta_1, \cdots, \theta_{n+2}$ such that the function $u(t)$ given by* (1.3) *satisfies* (1.2) *if and only if*

$$C(p_i, q_i, p_{i+1}, q_{i+1}, p_{i+2}, q_{i+2}) \times C(p_{i+1}, q_{i+1}, p_{i+2}, q_{i+2}, p_{i+3}, q_{i+3}) > 0, \quad (2.12)$$

for some $i \in \{1, \cdots, n+1\}$.

Now we can easily check the existence of the solution of equation (1.2) when $I = J-2$ by Theorem 2.1.7. However, this theorem cannot guarantee the uniqueness of t_i, parameters θ_i and a solution $u(t)$. By formulating a proper optimization problem, we introduce an meaningful algorithm to determine parameter function and its corresponding solution $u(t)$.

2.2 An algorithm for parameter function estimation

In this section we introduce an algorithm to estimate a piecewise constant parameter function in the case of $I < J - 1$. If information of input (Data points, number of subintervals and a structure of the subinterval is given, then the entire interval can be divided into several subgroups, which are either the form of T1 or T2. As we mentioned before, we perform the modified C-test only on T1 because the existence is always guaranteed in the case of T2. If the modified C-test fails, we cannot guarantee the existence of t_i and θ_i so we should choose another structure of the subintervals. Let us assume that the modified C-test succeed in T1. We can find t_i by minimizing the total variation of constant parameters θ_i in the whole interval. To do that, our objective functional can be defined by

$$f(t_1, \cdots, t_{n-1}) = \sum_{i=1}^{n-1} (\theta_{i-1} - \theta_i)^2, \tag{2.13}$$

where θ_i is a constant parameter in the subinterval depending on $\{t_i\}_{i=1}^{n-1}$. Here, n is the number of intervals in T1 or T2. And we have the following inequality constraints for the form of T1(see Figure 2.3).

$$p_1 < p_2 \le t_1 \le p_3 \le t_2 \le \cdots \le t_{n-2} \le p_n \le t_{n-1} \le p_{n+1} < p_{n+2}. \tag{2.14}$$

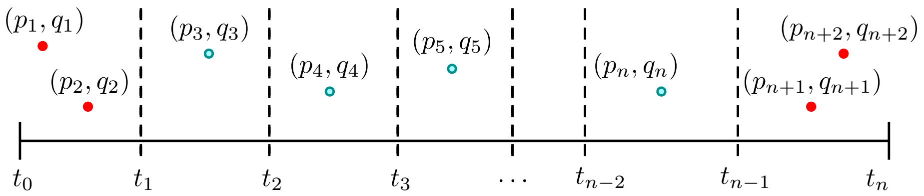


Figure 2.3: Each of the first and last intervals contains two data points and each of the others contains only one data point (T1).

Since t_{n-1} can be expressed uniquely in terms of $(t_{n-2}, u(t_{n-2}))$, (p_n, q_n), (p_{n+1}, q_{n+1}) and (p_{n+2}, q_{n+2}), the domain variables of the functional (2.13) can be reduced by one. Then the explicit formulation for the functional f can be rewritten as follows:

$$\begin{aligned} f(t_1, \cdots, t_{n-2}) =& \left(\frac{\log q_1 - \log q_2}{p_1 - p_2} - \frac{\log u(t_1) - \log q_1}{t_1 - p_1} \right)^2 \\ &+ \sum_{j=1}^{n-3} \left(\frac{\log u(t_j) - \log q_{j+2}}{t_j - p_{j+2}} - \frac{\log u(t_{j+1}) - \log q_{j+3}}{t_{j+1} - p_{j+3}} \right)^2 \\ &+ \left(\frac{\log u(t_{n-2}) - \log q_n}{t_{n-2} - p_n} - \frac{\log q_{n+1} - \log q_{n+2}}{p_{n+1} - p_{n+2}} \right)^2, \end{aligned}$$

where

$$u(t_1) = q_1 \exp\left\{\frac{\log q_1 - \log q_2}{p_1 - p_2}(t_1 - p_1)\right\}$$
$$= q_2 \exp\left\{\frac{\log q_1 - \log q_2}{p_1 - p_2}(t_1 - p_2)\right\},$$

and

$$u(t_k) = q_{k+1} \exp\left\{\frac{\log u(t_{k-1}) - \log q_{k+1}}{t_{k-1} - p_{k+1}}(t_k - p_{k+1})\right\}$$

for $k = 2, \cdots, n-2$. Combining these recursive relationships, we have

$$\begin{aligned}
\log u(t_k) =& \frac{t_k - p_{k+1}}{t_{k-1} - p_{k+1}} \log u(t_{k-1}) - \frac{t_k - t_{k-1}}{t_{k-1} - p_{k+1}} \log q_{k+1} \\
=& \frac{t_k - p_{k+1}}{t_{k-1} - p_{k+1}} \left\{ \frac{t_{k-1} - p_k}{t_{k-2} - p_k} \log u(t_{k-2}) - \frac{t_{k-1} - t_{k-2}}{t_{k-2} - p_k} \log q_k \right\} \\
& + \frac{t_k - t_{k-1}}{t_{k-1} - p_{k+1}} \log q_{k+1} \\
=& \cdots \\
=& \frac{(t_k - p_{k+1}) \cdots (t_2 - p_3)}{(t_{k-1} - p_{k+1}) \cdots (t_1 - p_3)} \log u(t_1) \\
& - \frac{(t_k - p_{k+1}) \cdots (t_3 - p_4)(t_2 - t_1)}{(t_{k-1} - p_{k+1}) \cdots (t_1 - p_3)} \log q_3 \\
& - \cdots - \frac{(t_k - p_{k+1})(t_{k-1} - t_{k-2})}{(t_{k-1} - p_{k+1})(t_{k-2} - p_k)} \log q_k \\
& - \frac{t_k - t_{k-1}}{t_{k-1} - p_{k+1}} \log q_{k+1}
\end{aligned}$$

This result implies that the term $u(t_k)$ can be represented by time nodes $\{t_i\}_{i=1}^k$ and data points.

In a similar manner, the constraint $p_n \leq t_{n-1} \leq p_{n+1}$ in the condition (2.14) can be expressed, for the variables $t_1, \cdots, t_{n-2}$, as

$$\left(\frac{\log q_n - \log q_{n+1}}{p_n - p_{n+1}} - \frac{\log q_{n+1} - \log q_{n+2}}{p_{n+1} - p_{n+2}}\right)\left(\frac{\log q_n - \log q_{n+1}}{p_n - p_{n+1}} - \frac{\log u(t_{n-2}) - \log q_n}{t_{n-2} - p_n}\right) \leq 0.$$

This is obtained by applying Proposition 2.1.5 to the following set

$$\{(t_{n-2}, u(t_{n-2})), (p_n, q_n), (p_{n+1}, q_{n+1}), (p_{n+2}, q_{n+2})\}.$$

Remark 2.2.1. *In T2 case, the objective functional* (2.13) *can be written*

$$\begin{aligned} f(t_1, \cdots, t_{n-1}) =& \left(\frac{\log q_1 - \log q_2}{p_1 - p_2} - \frac{\log u(t_1) - \log q_3}{t_1 - p_3} \right)^2 \\ &+ \sum_{j=1}^{n-2} \left(\frac{\log u(t_j) - \log q_{j+2}}{t_j - p_{j+2}} - \frac{\log u(t_{j+1}) - \log q_{j+3}}{t_{j+1} - p_{j+3}} \right)^2, \end{aligned}$$

where the first interval contains two data points and the others contain only one data point with inequality constraints

$$p_1 < p_2 \leq t_1 \leq p_3 \leq t_2 \leq \cdots \leq t_{n-1} \leq p_{n+1}.$$

Otherwise the objective functional (2.13) *can be written*

$$\begin{aligned} f(t_1, \cdots, t_{n-1}) =& \left(\frac{\log q_1 - \log q_2}{p_1 - p_2} - \frac{\log u(t_1) - \log q_3}{t_1 - p_3} \right)^2 \\ &+ \sum_{j=1}^{n-2} \left(\frac{\log u(t_j) - \log q_{j+2}}{t_j - p_{j+2}} - \frac{\log u(t_{j+1}) - \log q_{j+3}}{t_{j+1} - p_{j+3}} \right)^2, \end{aligned}$$

where the last interval contains two data points and the others contain only one data point with inequality constraints

$$p_1 < p_2 \leq t_1 \leq p_3 \leq t_2 \leq \cdots \leq t_{n-1} \leq p_{n+1}.$$

We use the numerical method proposed by Rockafellar [14] to find $\{t_i\}_{i=1}^{I-1}$ which minimize the objective functional subject to the inequality constraints. Let us introduce our algorithm in brief (See Algorithm 1).

Algorithm 1

Require: Data points, number of subintervals and structure of the subintervals.

Divide the whole interval into subgroups of the form T1 or T2

for all T1 cases **do**

  perform the modified C-test

  if the modified C-test fails **then**

    stop (Error : Existence is not guaranteed!)

  end if

end for

Find t_i which minimize the objective functional (2.13) with proper constraints

Find the parameters and its corresponding solution $u(t)$ of (1.2)

Chapter 3

Numerical Simulations

3.1 Data set 1

In data set 1, we deal with a set of ten data points which are listed in Table 3.1.

j	1	2	3	4	5	6	7	8	9	10
p_j	0.10	0.20	0.25	0.30	0.45	0.55	0.60	0.85	0.75	0.90
q_j	5.46	13.87	21.86	34.03	110.53	195.22	238.65	356.29	329.98	363.17

Table 3.1: Simulated data in Data Set 1

These data points are generated from the analytic solution to the following logistic differential equation.

$$\frac{du}{dt} = ru\left(1 - \frac{u}{K}\right), \quad t \in (p_1, p_{10}),$$
$$u(p_1) = u_0.$$

where the parameters $K = 375$, $r = 9.547976955$ and $u_0 = 2.121772657$ are taken from [8]. Note that this is positively well-posed data set.

Our goal of this paper is to find a piecewise parameter function to the ODE (1.2) which minimize the function (2.13). Before we proceed we should choose an one proper set of number of subintervals and a structure of the subinterval. Since we consider ten data points, the proper number of subinterval I is in a range from 5 to 9. If I is less than 5, it goes against to the definition of irreducible data set. Also if I is greater than 9, its subinterval contains only one or zero data point and this does not reflect on the dependency of data points properly. From this reason, we may select a number $I \in \{5, 6, 7, 8, 9\}$.

In this example, let us assume that the number of subintervals is seven, that is, $I = 7$ and the structure of subinterval is (2, 2, 1, 1, 1, 1, 2) which means the first, second and seventh interval have two data points and the other has one data point. As illustrated in Figure 3.1, the whole interval is composed of two subgroups (G1 and G2) that is rectangled to identify which data points belong to which subgroup. This decomposition is based on Lemma 1.3.2 to determine parameter uniquely by using two data points in one subinterval.

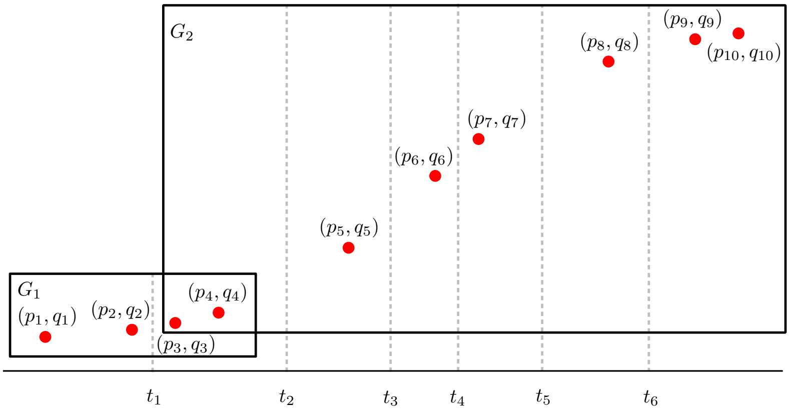


Figure 3.1: A given information of data set 1

First, let us consider the subgroup G1. Note that this subgroup, which has two subintervals, is classified as T1. According to Algorithm 1, we need to perform the modified C-test for G1. From the simple evaluation

$$C(p_1, q_1, p_2, q_2, p_3, q_3) \times C(p_2, q_2, p_3, q_3, p_4, q_4) = 6.8894 \times 10^{-7} > 0,$$

we know that there exist t_1, θ_1 and θ_2 to a solution $u(t)$ of the equation (1.2) as shown in Proposition 2.1.5.

Similarly, the second group G2, which has six subintervals, is classified as T1.Here, of course, two data points (p_3, q_3) and (p_4, q_4) are common elements of G1 and G2. The subgroup G2 is also T1, so we need to perform the modified C-test again. Since

$$C(p_4, q_4, p_5, q_5, p_6, q_6) \times C(p_5, q_5, p_6, q_6, p_7, q_7) = 2.7138 \times 10^{-7} > 0,$$

the existence of time nodes and parameters in G2 is ensured. Now we can go further with the success of the modified C-test and can get the results shown in Table 3.2 and Table 3.3 by applying a numerical scheme to minimize the functional (2.13).

t_0	t_1	t_2	t_3	t_4	t_5	t_6	t_7
0.10000	0.22691	0.36204	0.46342	0.55737	0.60754	0.77273	0.90000

Table 3.2: The minimization results of the functional (2.13) for the data set 1

θ_1	θ_2	θ_3	θ_4	θ_5	θ_6	θ_7
9.31914	8.84667	7.15449	5.46094	3.76750	2.07546	0.38248

Table 3.3: The numerical value of parameters of the equation (1.2) for the data set 1

With estimated time nodes and parameters, the L_2 error between numerical solution and exact solution of (1.2) is 1.7055×10^{-2} and the graph of the solution is shown in Figure 3.2.

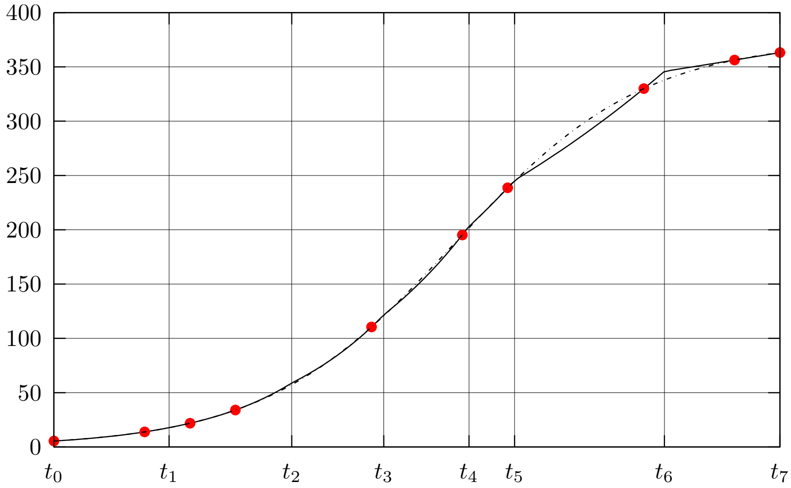


Figure 3.2: The dashed line is the exact solution of (1.2), and the solid line is the numerical solution. Dots represent data points.

3.2 Data set 2

In data set 2, we generate $\{p_j\}_{j=1}^{10}$ as random numbers in $[-1, 1]$ and $\{q_j\}_{j=1}^{10}$ by solving the following differential equation at p_j.

$$\frac{du}{dt} = t^2 u, \quad t \in (p_1, p_{10});$$
$$u(p_1) = e^{p_1^3/3}.$$

The generated data set $\{(p_j, q_j)\}_{j=1}^{10}$ are listed in Table 3.4. For data set 2, we

j	1	2	3	4	5	6	7	8	9	10
p_j	-0.90	-0.75	-0.55	-0.45	-0.20	0.00	0.25	0.30	0.60	0.85
q_j	0.7843	0.8688	0.9461	0.9701	0.9973	1.00	1.0052	1.0090	1.0747	1.2272

Table 3.4: Simulated data in Data Set 2

consider the seven subinterval with $I = 7$ and the structure of subinterval is (1, 1, 1, 2, 2, 1, 2). In other words, the fourth, fifth and seventh subinterval have two data points and the other has one data point. As depicted in Figure

3.3, the whole interval can be decomposed by three subgroups G1, G2 and G3.

The first subgroup G1, which has four subintervals, is classified as T2.In this case, we don't need to perform the modified C-test since it is T2, and thus the existence of time nodes and its corresponding parameters are always guaranteed.

On the other hand, G2 and G3 have respectively two and three subintervals and both of them is classified as T1. Thus we should perform the modified C-test. In G2, however, we get a negative value of

$$C(p_4, q_4, p_5, q_5, p_6, q_6) \times C(p_5, q_5, p_6, q_6, p_7, q_7) = -1.8281 \times 10^{-6}$$

and this implies non-existence of t_4 of the equation (1.2). Accordingly, we cannot determine a piecewise constant parameter function $\theta(t)$ which satisfies (1.2) with data set 2.

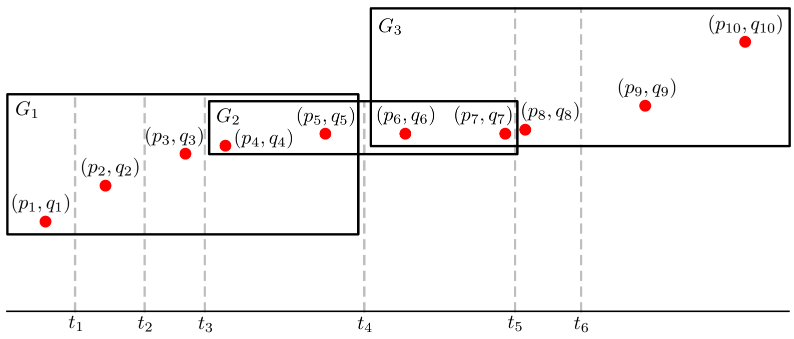


Figure 3.3: A given information of data set 2; dots represent data points.

Let us consider another data set. Suppose now that the seven subinterval with $I = 7$ is given and the structure of subinterval is (1, 1, 2, 1, 2, 1, 2). In this case, the third, fifth and seventh subinterval have two data points and the other has one data point. And the whole interval can be decomposed by three subgroups G1, G2 and G3. Like other data sets, we need to perform the modified C-test for G2 and G3 which are T1. And from the simple calculations, we can find that the modified C-test is successful. Based on this fact, we can calculate the optimal parameter function and the results are listed in Table 3.5 and Table 3.6. Also the L_2 error between numerical solution and exact solution of (1.2) is 4.9836×10^{-3}.

t_0	t_1	t_2	t_3	t_4	t_5	t_6	t_7
-0.90000	-0.75750	-0.59574	-0.34737	-0.00000	0.28494	0.59400	0.85000

Table 3.5: The minimization results of the functional (2.13).

θ_1	θ_2	θ_3	θ_4	θ_5	θ_6	θ_7
0.69334	0.47768	0.25085	0.013339	0.020822	0.20346	0.53083

Table 3.6: The numerical value of parameters of the equation (1.2).

3.3 Details of calculation in Lemma 2.1.6

$$
\begin{aligned}
f(p_2,p_3) =& \left[\frac{\log q_1-\log q_2}{p_1-p_2}-\frac{\log q_4-\log q_5}{p_4-p_5}\right]p_2p_3\\
&-\left[\frac{\log q_1-\log q_2}{p_1-p_2}p_3-\log q_3+\frac{p_4\log q_5-p_5\log q_4}{p_4-p_5}\right]p_2\\
&+\left[\frac{p_1\log q_2-p_2\log q_1}{p_1-p_2}-\log q_3+\frac{\log q_4-\log q_5}{p_4-p_5}p_3\right]p_3\\
&-\left[\frac{p_1\log q_2-p_2\log q_1}{p_1-p_2}-\frac{p_4\log q_5-p_5\log q_4}{p_4-p_5}\right]p_3\\
=&\frac{p_2p_3-p_2p_3-p_2p_3+p_2p_3}{p_1-p_2}\log q_1\\
&-\frac{p_2p_3-p_2p_3-p_1p_3-p_1p_3}{p_1-p_2}\log q_2\\
&-(p_3-p_2)\log q_3\\
&-\frac{p_2p_3-p_2p_5-p_3^2+p_3p_5}{p_4-p_5}\log q_4\\
&+\frac{p_2p_3-p_2p_4-p_3^2+p_3p_4}{p_4-p_5}\log q_5\\
=&(p_2-p_3)\log q_3-\frac{(p_2-p_3)(p_3-p_5)}{p_4-p_5}\log q_4\\
&+\frac{(p_2-p_3)(p_3-p_4)}{p_4-p_5}\log q_5\\
=&\frac{p_2-p_3}{p_4-p_5}\times C(p_3,q_3,p_4,q_4,p_5,q_5),
\end{aligned}
$$

$$
\begin{aligned}
f(p_2,p_4) =& \left[\frac{\log q_1 - \log q_2}{p_1 - p_2} - \frac{\log q_4 - \log q_5}{p_4 - p_5}\right] p_2 p_4 \\
& - \left[\frac{\log q_1 - \log q_2}{p_1 - p_2} p_3 - \log q_3 + \frac{p_4 \log q_5 - p_5 \log q_4}{p_4 - p_5}\right] p_2 \\
& + \left[\frac{p_1 \log q_2 - p_2 \log q_1}{p_1 - p_2} - \log q_3 + \frac{\log q_4 - \log q_5}{p_4 - p_5} p_3\right] p_4 \\
& - \left[\frac{p_1 \log q_2 - p_2 \log q_1}{p_1 - p_2} - \frac{p_4 \log q_5 - p_5 \log q_4}{p_4 - p_5}\right] p_3 \\
=& \frac{p_2 p_4 - p_2 p_3 - p_2 p_4 + p_2 p_3}{p_1 - p_2} \log q_1 \\
& - \frac{p_2 p_4 - p_2 p_3 - p_1 p_4 + p_1 p_3}{p_1 - p_2} \log q_2 \\
& - (p_4 - p_2) \log q_3 \\
& - \frac{p_2 p_4 - p_2 p_5 - p_3 p_4 + p_3 p_5}{p_4 - p_5} \log q_4 \\
& + \frac{p_2 p_4 - p_2 p_4 - p_3 p_4 + p_3 p_4}{p_4 - p_5} \log q_5 \\
=& - (p_3 - p_4) \log q_2 - (p_4 - p_2) \log q_3 - (p_2 - p_3) \log q_4 \\
=& - C(p_2, q_2, p_3, q_3, p_4, q_4),
\end{aligned}
$$

$$
\begin{aligned}
f(p_3,p_4) =& \left[\frac{\log q_1 - \log q_2}{p_1 - p_2} - \frac{\log q_4 - \log q_5}{p_4 - p_5}\right] p_3 p_4 \\
& - \left[\frac{\log q_1 - \log q_2}{p_1 - p_2} p_3 - \log q_3 + \frac{p_4 \log q_5 - p_5 \log q_4}{p_4 - p_5}\right] p_3 \\
& + \left[\frac{p_1 \log q_2 - p_2 \log q_1}{p_1 - p_2} - \log q_3 + \frac{\log q_4 - \log q_5}{p_4 - p_5} p_3\right] p_4 \\
& - \left[\frac{p_1 \log q_2 - p_2 \log q_1}{p_1 - p_2} - \frac{p_4 \log q_5 - p_5 \log q_4}{p_4 - p_5}\right] p_3 \\
=& \frac{p_3 p_4 - p_3^2 - p_2 p_4 + p_2 p_3}{p_1 - p_2} \log q_1 \\
& - \frac{p_3 p_4 - p_3^2 - p_1 p_4 + p_1 p_3}{p_1 - p_2} \log q_2 \\
& - (p_4 - p_3) \log q_3 \\
& - \frac{p_3 p_4 - p_3 p_5 - p_3 p_4 + p_3 p_5}{p_4 - p_5} \log q_4 \\
& + \frac{p_3 p_4 - p_3 p_4 - p_3 p_4 + p_3 p_4}{p_4 - p_5} \log q_5 \\
=& \frac{(p_2 - p_3)(p_3 - p_4)}{p_1 - p_2} \log q_1 - \frac{(p_1 - p_3)(p_3 - p_4)}{p_1 - p_2} \log q_2 \\
& + (p_3 - p_4) \log q_3 \\
=& \frac{p_3 - p_4}{p_1 - p_2} \times C(p_1, q_1, p_2, q_2, p_3, q_3).
\end{aligned}
$$

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Part II

Facility Location Problem

Chapter 4

Introduction

The purpose of this part is to suggest a closed solution algorithm for finding a circle which passes through two fixed points and the maximum of distance from the circle to a set of given points is minimized. This sort of constrained minimax problems occur for instance in the design of round printed circuit boards (PCBs).

PCB is also referred as printed wiring board (PWB) or etching wiring board. Usually a computer aided design (CAD) software is used for designing electronic circuit schematics and layouts. The schematic of a circuit is a sketch of how different electronic components are connected together. This schematic is then converted into a layout, which is the actual image of the circuit as it will appear on the Printed Circuit Board (PCB). Usually, rectangular shaped layouts are made, but there are several cases where round shapes are in preference, for instance, in designing light-emitting diod (LED) and other circular shaped boards.

Recently PC boards tend to have more complex structure, and thus more elaborate manufacturing systems are required [2]. Typically the design of PC boards is performed with computer integrated manufacturing systems and equipment, and it is one of the most important computer aided manufacturing(CAM) examples [11, 12]. Efficient circuit designs depend on how to locate nodes and how to connect geometrically nodes that are supposed to be connected. Once the set of nodes that need to be interconnected is given, the connection is performed by using line and circular elements, in order to minimize any errors in the chemical etching process. Usually such a set of nodes is supposed to be connected to two extra fixed nodes. Also, it is very important to have the number of connecting arcs and lines as small as possible. In connecting all the nodes that are supposed to be connected, in order to maximize efficiency in the etching process, a circular arc which passes through two fixed nodes is determined, and then line segments from nodes to the circular arc will be connected to complete the whole process. Here, one should choose a circular arc such that the maximum length of line segments is as minimal as possible. This factor is critically related to the efficiency of PC board design.

We now formulate the above problem mathematically. Consider the set of data points in the plane $\mathbf{P_j}(x_j, y_j)$, $j = 1, \cdots, n$ and two additional points $\mathbf{Q_1}$ and $\mathbf{Q_2}$ which are distinct from $\mathbf{P_j}$, $j = 1, \cdots, n$. And let w_j denote the weight corresponding to the data point $\mathbf{P_j}$ for all $j = 1, \cdots, n$. We are interested in the *constrained optimization problem* of finding a circle that is closest to the set of points $\mathbf{P_j}$, $j = 1, \cdots, n$, among all the circles that are constrained to pass through $\mathbf{Q_1}$ and $\mathbf{Q_2}$ (see Figure 4.1 for the suggested problem setting). To measure the closeness between a circle and a set of points, we define the distance function as

$$d_j(\mathbf{X}) = \|\mathbf{P_j} - \mathbf{X}\|_2 - \|\mathbf{Q_1} - \mathbf{X}\|_2.$$

where $\|\cdot\|_p$ denotes the ℓ^p-norm for $1 \le p \le \infty$ and let w_j denote the weight corresponding to the data point $\mathbf{P_j}$ for all $j = 1, \cdots, n$.

Now our *constrained optimization problem* can be written as follows : find $\mathbf{X} \in \mathbb{R}^2$ which minimizes

$$\max_j w_j |d_j(\mathbf{X})| \quad \text{subject to } \|\mathbf{Q_1} - \mathbf{X}\|_2 - \|\mathbf{Q_2} - \mathbf{X}\|_2 = 0. \tag{4.1}$$

For the design of usual PCBs, all the weights are equal. But, in this work, we consider the weighted distance function in order to enable to reflect different features of materials that might be necessary for the design of some manufacturing systems.

A class of similar problems to (4.1) has a long history of developments. Drezner[4] proposed an algorithm for the problem

$$\operatorname*{arg\,min}_{X \in \mathbb{R}^2,\ R>0} \|(d_1(\mathbf{X}), d_2(\mathbf{X}), \cdots, d_n(\mathbf{X}))\|_p \quad (p = 1, 2 \text{ and } \infty).$$

Nonlinear minimax problems with successive approximation methods for finding a stationary point are also studied by Demjanov [5]. The concept of controlling fitting circles are used: Gass *et al.*[7, 8, 9] suggest some algorithms to solve squared difference problems by using dual methods. Also, Brimberg *et al.*[3] introduced an algorithm for finding an optimal location which minimizes the longest Euclidean distance between the circle and facility data.

In this thesis, as described in the beginning of the section, we restrict to the optimization problem of finding a circle which passes through two given points. We propose a systematic approach to resolve this minimax problems, obtaining an exact optimum solution.

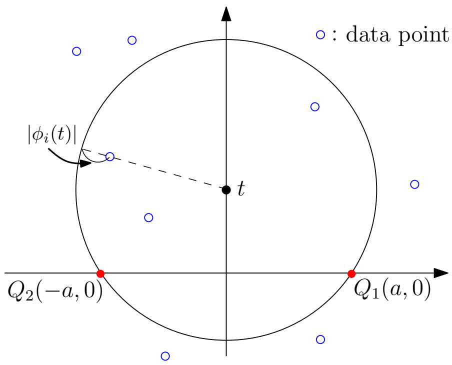


Figure 4.1: The constrained optimization problem of finding a circle that is closest to all points among all the circles that are constrained to pass through $\mathbf{Q_1}$ and $\mathbf{Q_2}$.

Chapter 5

The nonlinear minimax problem

In this section, we introduce an algorithm for solving the minimax problem (4.1) by transforming this to an *unconstrained minimax problem*. Moreover we describe an explanation on how it works.

5.1 Reformulation of the minimax problem

Without loss of generality, we can assume that $\mathbf{Q_1} = (a, 0)$ and $\mathbf{Q_2} = (-a, 0)$ for some positive number $a > 0$. Then the problem of finding a circle, passing through two points $\mathbf{Q_1}$ and $\mathbf{Q_2}$, requires that the center be located on the perpendicular bisector (y-axis) of the line segment $\mathbf{Q_1Q_2}$ (see Figure 4.1). Then Problem (4.1) can be reformulated as the following one-dimensional optimization problem : Find a point $X^* = (0, t^*)$ which minimizes

$$\phi(t) := \max_j \phi_j(t) \tag{5.1}$$

where $\phi_j(t) := w_j \left| d_j(\mathbf{X}) \right| = w_j \left| \sqrt{x_j^2 + (t - y_j)^2} - \sqrt{t^2 + a^2} \right|$ with $\mathbf{X} = (0, t)$. Here, $\sqrt{x_j^2 + (t - y_j)^2}$ means the distance between the data point $\mathbf{P_j}$ and the center of the circle and $\sqrt{t^2 + a^2}$ means the radius of the circle. It is called a minimax problem and cannot be solved directly by using a usual gradient methods. Indeed, difficulty occurs where the max function and/or the absolute function is not differentiable.

Now we start with finding candidates for the optimum of the given minimax problem (5.1).

Lemma 5.1.1. *Suppose that there does not exist a circle which passes through* $\mathbf{Q_1}$*,*$\mathbf{Q_2}$ *and the data points* $\mathbf{P_j}$*,* $j = 1, \cdots, n$*. Then the local minimum of Problem* (5.1) *are at the intersection point of the graphs* $y = \phi_{k_1}(t)$ *and* $y = \phi_{k_2}(t)$ *for some distinct integers* k_1 *and* k_2*.*

Proof. Suppose that the function $\phi(t)$ has a local minimum at a point t' which is not an intersection point of two distinct functions $\phi_{k_1}(t)$ and $\phi_{k_2}(t)$. Since $\phi(t)$ is a piecewise smooth function, there should exist some j and a sufficiently small positive ϵ such that $\phi(t) = \phi_j(t)$ on $(t' - \epsilon, t' + \epsilon)$. Then we know the fact that t' is a critical point of ϕ, and thus must be a critical point of ϕ_j thereon (see Figure 5.1 for instance). Since absolute valued functions are not differentiable at the points where the function vanishes, the critical points of ϕ_j are obtained from either

$$0 = \frac{\partial}{\partial t} d_j(t) = w_j \left(\frac{t - y_j}{\sqrt{x_j^2 + (t - y_j)^2}} - \frac{t}{\sqrt{t^2 + a^2}} \right),$$

in the case of $d_j(t) \neq 0$; or

$$d_j(t) = 0.$$

Thus the exact critical point t' of the function $\phi_j(t)$ should be either $t_\pm = \frac{a y_j}{a \pm x_j}$, or $t_0 = \frac{x_j^2+y_j^2-a^2}{2y_j}$. We treat the two cases separately.

i) If $t' = t_\pm$, then we have

$$d_j(t')d_j''(t') = -\frac{w_j^2(|a|-|x_j|)^2(a \pm x_j)^2}{|ax_j|} < 0.$$

This means that if $d_j(t')$ is positive then $d_j''(t')$ is negative, and thus d_j has a local maximum at t'. Similarly, if $d_j(t')$ is negative then $d_j''(t')$ is positive, and thus d_j has a local minimum at t'. By considering absolute value of the function d_j, we can conclude that t' is a local maximum point of the function ϕ. This contradicts our assumption that t' is a local minimum point.

ii) If $t' = t_0$, then $\phi(t') = \phi_j(t') = 0$. From the definition of the function $\phi(t)$, it is trivial that $\phi_k(t') = 0$ for all $k = 1, \cdots, n$. This means that there exist a circle which passes through $\mathbf{Q_1}$,$\mathbf{Q_2}$ and the data points $\mathbf{P_j}, j = 1, \cdots, n$. Thus it is a contradiction to the assumption.

Both cases i) and ii) lead to a contradiction to our assumption. Therefore, the local minimum of $\phi(t)$ must be taken at a point t' which is an intersection point of two functions $\phi_{k_1}(t)$ and $\phi_{k_2}(t)$ for some distinct integers k_1 and k_2. $\square$

A simple example of the Lemma 5.1.1 is shown in Figure 5.1. The local minima of $\phi := \max\{\phi_j, \phi_k\}$ are taken at the intersection points of $y = \phi_j(t)$ and $y = \phi_k(t)$. The lemma can be used to answer the question of where to place the center of the circle to solve Problem (5.1). In order to simplify the notation, we will use the following notation for the set of intersection points:

$$\mathcal{I} := \bigcup_{\substack{j,k=1 \\ j \neq k}}^{n} \{t \mid \phi_j(t) = \phi_k(t)\}.$$

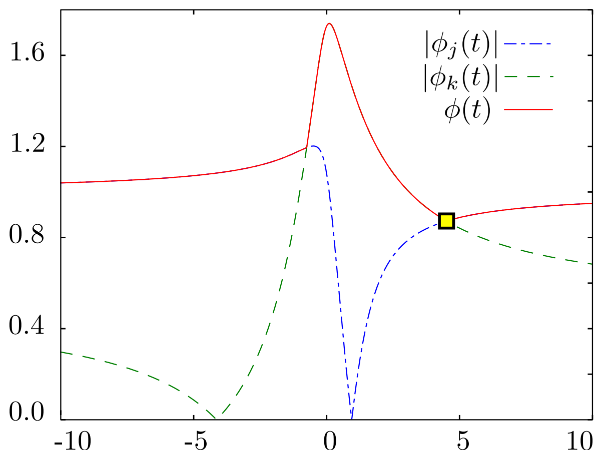


Figure 5.1: An example of graphs $y = \phi_j(t)$, $y = \phi_k(t)$ and $y = \phi(t) = \max\{\phi_j(t), \phi_k(t)\}$. A local minimum of $y = \phi(t)$ are taken at yellow marked square which are elements of the intersection points of $y = \phi_j(t)$ and $y = \phi_k(t)$. This plot is generated using the data points $(x_j, y_j) = (1, 1)$ and $(x_k, y_k) = (2, -0.5)$ when $a = 1/3$.

The next theorem follows from the above lemma.

Theorem 5.1.2. *Let t^* be a point such that*

$$\phi(t^*) = \min_{t \in \mathcal{I}} \phi(t).$$

If $\phi(t^*) \leq \max_j w_j |y_j|$, then $\phi(t^*)$ is a global minimum for Problem (5.1)*; otherwise, Problem* (5.1) *does not have a global minimum solution.*

Proof. Let us begin with finding the candidates of global minimum of $\phi(t)$ using the above Lemma 5.1.1. Since solving the equation $\phi_j(t) = \phi_k(t)$ is equivalent to solving the equation $\phi_j^2(t) = \phi_k^2(t)$, we can find the elements of the set $\mathcal{I}$ by solving

$$\begin{aligned} 0 &= \phi_j^2(t) - \phi_k^2(t) \\ &= \left(w_j\sqrt{x_j^2 + (t-y_j)^2} - w_k\sqrt{x_k^2 + (t-y_k)^2} - (w_j - w_k)\sqrt{t^2 + a^2}\right) \\ &\quad \times \left(w_j\sqrt{x_j^2 + (t-y_j)^2} + w_k\sqrt{x_k^2 + (t-y_k)^2} - (w_j + w_k)\sqrt{t^2 + 0a^2}\right) \\ &=: I_1^w(t) \times I_2^w(t). \end{aligned} \tag{5.2}$$

Equation (5.2) is divided into $I_1^w(t) = 0$ or $I_2^w(t) = 0$. To solve the equation $I_1^w(t) = 0$, move the radical term $(w_j - w_k)\sqrt{t^2 + a^2}$ to the right side of the equation and square both sides. Then we get

$$\begin{aligned} &(w_j^2 + w_k^2)t^2 - 2(w_j^2 y_j + w_k^2 y_k)t + \{w_j^2(x_j^2 + y_j^2) + w_k^2(x_k^2 + x_k^2)\} \\ &\qquad - 2w_j w_k\sqrt{x_j^2 + (t-y_j)^2}\sqrt{x_k^2 + (t-y_k)^2} \\ &= (w_j - w_k)^2(t^2 + a^2). \end{aligned}$$

To isolate the radical expression to the left side, move all the other terms to the right and square both sides of the equation again. Then one gets the following cubic polynomial equation:

$$p_{jk}(t) = a_0 t^3 + a_1 t^2 + a_2 t + a_3 = 0, \tag{5.3}$$

where

$$
\begin{aligned}
a_0 &= 8w_jw_k(w_j - w_k)(w_jy_j - w_ky_k),\\
a_1 &= -4\bigl[\{w_j^2(x_j^2 + y_j^2 - a^2) + 2w_jw_ka^2 + w_k^2(x_k^2 + y_k^2 - a^2)\}w_jw_k\\
&\qquad + (w_j^2y_j + w_k^2y_k)^2 - w_j^2w_k^2\{x_j^2 + y_j^2 + x_k^2 + y_k^2 + 4y_jy_k\}\bigr],\\
a_2 &= 4\{w_j^2(x_j^2 + y_j^2 - a^2) + 2w_jw_ka^2 + w_k^2(x_k^2 + y_k^2 - a^2)\}(w_j^2y_j + w_k^2y_k)\\
&\qquad + 8w_j^2w_k^2\{(x_j^2 + y_j^2)y_k + (x_k^2 + y_k^2)y_j\},\\
a_3 &= -\{w_j^2(x_j^2 + y_j^2 - a^2) + 2a^2w_jw_k + w_k^2(x_k^2 + y_k^2 - a^2)\}^2\\
&\qquad\qquad - 4w_j^2w_k^2(x_j^2 + y_j^2)(x_k^2 + y_k^2).
\end{aligned}
$$

Similarly, solving the equation $I_2^w(t) = 0$ is equivalent to solving the following cubic polynomial equation:

$$q_{jk}(t) = b_0t^3 + b_1t^2 + b_2t + b_3 = 0,$$

where

$$
\begin{aligned}
b_0 &= 8w_jw_k(w_j + w_k)(w_jy_j + w_ky_k),\\
b_1 &= -4\bigl[\{w_j^2(x_j^2 + y_j^2 - a^2) - 2w_jw_ka^2 + w_k^2(x_k^2 + y_k^2 - a^2)\}w_jw_k\\
&\qquad - (w_j^2y_j + w_k^2y_k)^2 + w_j^2w_k^2\{x_j^2 + y_j^2 + x_k^2 + y_k^2 + 4y_jy_k\}\bigr],\\
b_2 &= -4\{w_j^2(x_j^2 + y_j^2 - a^2) - 2w_jw_ka^2 + w_k^2(x_k^2 + y_k^2 - a^2)\}(w_j^2y_j + w_k^2y_k)\\
&\qquad + 8w_j^2w_k^2\{(x_j^2 + y_j^2)y_k + (x_k^2 + y_k^2)y_j\},\\
b_3 &= \{w_j^2(x_j^2 + y_j^2 - a^2) - 2w_jw_ka^2 + w_k^2(x_k^2 + y_k^2 - a^2)\}^2\\
&\qquad\qquad - 4w_j^2w_k^2(x_j^2 + y_j^2)(x_k^2 + y_k^2).
\end{aligned}
$$

By using Cardano's formula, one can find all the real roots of $p_{jk}(t)$ and $q_{jk}(t)$. In this way, one can find all the intersection points of $y = \phi_j(t)$ and

$y = \phi_k(t)$ for $j, k = 1, \cdots, n$. Then by comparing the values of the function $\phi(t)$ at these points, one can find the candidate of global minimum at t^*.

Of course, as the continuous function $\phi(t)$ is defined on a noncompact domain $\mathbb{R}$, the global minimum may not exist. However, using the expression

$$\phi_j(t) = \frac{w_j \left| x_j^2 + y_j^2 - a^2 - 2ty_j \right|}{\sqrt{x_j^2 + (t - y_j)^2} + \sqrt{t^2 + a^2}},$$

we have $\phi(t) \to \max_j w_j |y_j|$ as $t \to \pm\infty$. Thus if $\phi(t^*) \leq \max_j w_j |y_j|$, then $\phi(t^*)$ is a global minimum. If $\phi(t^*) > \max_j w_j |y_j|$, then the function $\phi(t)$ does not have global minimum. This completes the proof. $\square$

Remark 5.1.3. *If all the weights in* (4.1) *are equal, the roots of the equation* $I_1^w(t) = 0$ *in* (5.2) *can be given explicitly as* $t = \frac{x_j^2 - x_k^2 + y_j^2 - y_k^2}{2(y_j - y_k)}$, *instead of solving the cubic polynomial equation* (5.3). *This enables to find the elements of the set* $\mathcal{I}$ *roughly at a half computing cost.*

Example 5.1.4. *Suppose that we are given* $a = 1/3$ *and a set of three points* $\{(2, -\frac{1}{2}), (1, -1), (1, 1)\}$. *For notational simplicity, let us denote by* $\phi_{(p,q)}(t)$ *the distance between a given data point* (p, q) *and the circle at center* $(0, t)$ *with radius* $\sqrt{t^2 + a^2}$. *Then one can find five intersection points of* $y = \phi_{(2,-0.5)}(t)$, $y = \phi_{(1,-1)}(t)$ *and* $y = \phi_{(1,1)}(t)$ *as shown in Figure 5.2. Since the value of the function* $\phi(t)$ *approaches 1 as* t *goes to infinity and* $\phi(t)$ *is greater than 1 at these intersection points, none of these intersection points is optimal. This means that the function* $\phi(t)$ *has optimal value when* t *is infinity and this can be interpreted as a circle with radius infinity. It describes the straight line* $y = t$ *which passes through the points* $(\pm a, 0)$.

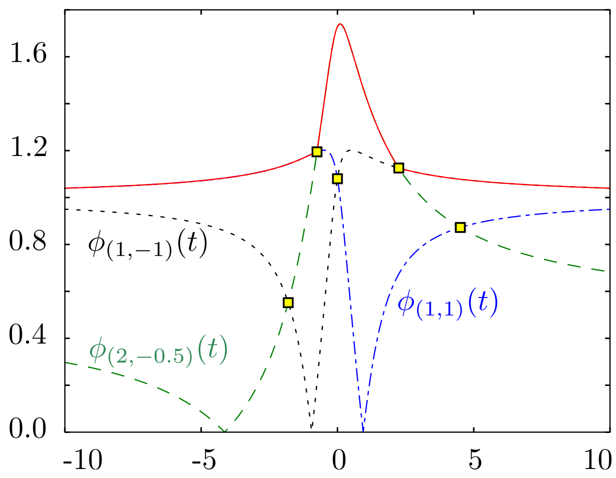


Figure 5.2: This is a description of the Example 5.1.4. The solid red curve represent the graph of the function $y = \phi(t)$ in (5.1). Also five yellow squares are marked to show intersection points of three distance functions $\phi_{(2,-0.5)}(t)$, $\phi_{(1,-1)}(t)$ and $\phi_{(1,1)}(t)$.

5.1.1 Algorithm for the location of a circle

Summarizing the above procedure in the proof of Theorem 5.1.2, we propose Algorithm 2 for solving the minimax problem (4.1) or (5.1).

5.1.2 Computational complexity

We will discuss efficiency of Algorithm 2 to find the location of a circle with increasing number of points $\mathbf{P_j}$'s. Since the number of intersection points increases at a rate of $\binom{n}{2}$ as n increases, finding all elements of the set $\mathcal{I}$ costs the computational complexity of $\mathrm{O}(n^2)$ at line 8 of the algorithm. Also the time to compute $\phi(t)$ for each $t \in \mathcal{I}$ costs $\mathcal{O}(n)$. Thus its overall complexity is $\mathcal{O}(n^3)$ at line 10 of the algorithm.

Algorithm 2 Algorithm for the location of a circle

$a \leftarrow \overline{\mathbf{Q_1 Q_2}}/2$
choose the proper coordinates system such that $\mathbf{Q_1} = (a, 0)$ and $\mathbf{Q_2} = (-a, 0)$
if $\mathbf{Q_1}$, $\mathbf{Q_2}$ and $\mathbf{P_j}$, $j = 1, \cdots, n$ are located on one specific circle **then**
    Global minimum is zero
else
    $\mathcal{I} \leftarrow \emptyset$
    for $j, k = 1, \cdots, n$ such that $j \neq k$ **do**
        $\mathcal{I} \leftarrow \mathcal{I} \cup \{t \,|\, \phi_j(t) = \phi_k(t)\}$
    end for
    Find t^* such that $\phi(t^*) = \min_{t \in \mathcal{I}} \phi(t)$
    if $\phi(t^*) \leq \max_j w_j |y_j|$ **then**
        $\phi(t^*)$ is the global minimum
    else
        the line through Q_1 and Q_2 is the global minimum
    end if
end if

Chapter 6

Numerical results

In this section we present and discuss some numerical results of our Algorithm 2. In order to verify stability of the numerical results, the algorithm is applied to a set of test cases.

In what follows, our experiments were run using F90/95. These are compiled with Intel Fortran Compiler in a SUSE Linux system with the architecture Intel i3 CPU 540 of 3.07 GHz chipset. Also we will assume that, unless otherwise stated, double precision formats are used.

6.1 Test case 1

In this subsection, we will consider some randomly generated data points with the aim of testing the hypothesis that Algorithm 2 finds the global minimizer to Problem (5.1) (see Table 6.1).

A simple calculation of the algorithm shows that the global minimizer of the problem is

$$(x^*, y^*) = (0.6986086149, 0.4165360718)$$

with the global minimum $\phi(t^*) = 0.1077162733$. And Figs. 6.1b and 6.1c also show that the result obtained by our algorithm is the correct global minimizer.

j	x_j	y_j	w_j
1	0.7274889350	0.8204632998	0.8016711473
2	0.2797133327	0.9459880590	0.2636268735
3	0.6873669028	0.2331188768	0.6819188595
4	0.5615428090	0.5534529090	0.3317854106
5	0.9512923360	0.4554860294	0.2297016978
6	0.09882796556	0.5339425206	0.2762681842
7	0.1414267719	0.3058254719	0.3449728787
8	0.5659797192	0.3396259248	0.9184667468
9	0.4611324966	0.6166244745	0.7779603601
10	0.7197866440	0.8820757270	0.3015199602

(a) A set of randomly chosen data $\{(x_j, y_j)\}_{j=1}^{10}$ with corresponding weights $w_j, j = 1, \cdots, 10$.

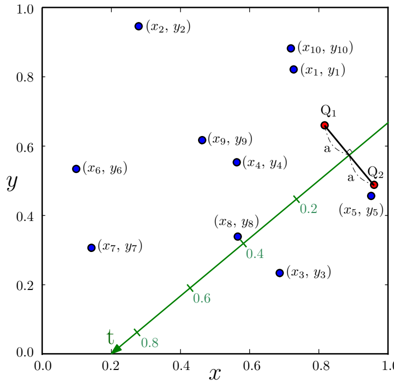
$\mathbf{Q_1}$	(0.8170491457, 0.6598317623)
$\mathbf{Q_2}$	(0.9594544172, 0.4885112047)

(b) Randomly chosen $\mathbf{Q_1}$ and $\mathbf{Q_2}$.

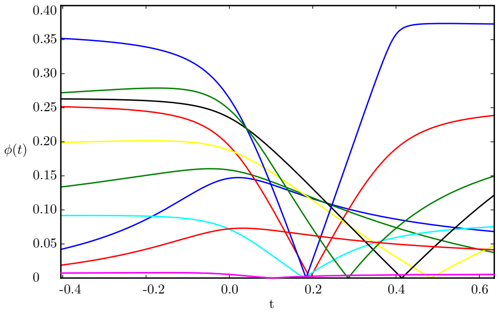
Table 6.1: Data set for test case 1

6.2 Test case 2

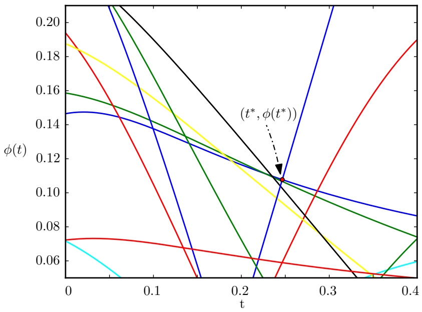
In this subsection, we provide one of the equivalent formulations of the minimax problem to verify the proposed algorithm.



(a) Plot of data set; The axis of coordinate in the interior represent t axis.



(b) Plot of $|\phi_j|$ functions restricted to the perpendicular bisector of the line $\mathbf{Q_1Q_2}$ (see the green line in Figure 6.1a).



(c) Expanded plot Figure 6.1b

Figure 6.1: Plots of data set in Table 6.1 and corresponding function ϕ_j's

Consider the following data set:

$$\{(x_j, y_j)\}_{j=1}^{N^2} = \left\{ \left(\left(\frac{N^2-1}{N^2}\right)^{l-1}, \left(\frac{N^2-1}{N^2}\right)^{m-1} \right) \middle| \, l, m = 1, \cdots, N \right\}, \tag{6.1}$$

and

$$a = 1/3,$$

for positive integer N which is equal to $\sqrt{n}$. All the weights are supposed to be equal to one, the plot of the data set can be shown as Figure 6.2.

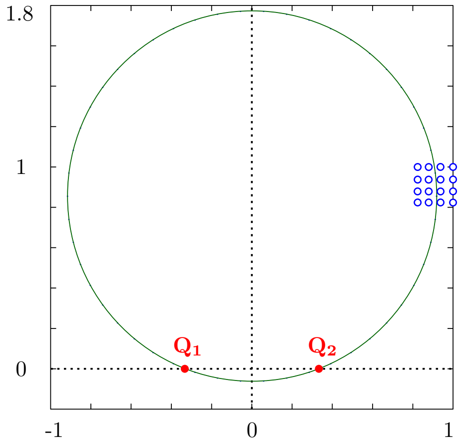


Figure 6.2: An example of data set (6.1) with 16 points ($n = 16$)

The numerical results obtained for the proposed Algorithm 2 to the above data set are summarized in Table 6.2, where "Time" and "It" mean the CPU time in seconds and the number of iterations, respectively. Table 6.2a presents the values of optimal variables obtained from Exflib (multiple precision arithmetic library) [6], which is a package to compute in arbitrary high precision. The numerical values using 100 digits computation are then formatted into strings to keep 20 significant digits. Table 6.2b presents the results of (standard) double precision computation. These indicate that the difference between the numerical solutions of a 100 digits computation and double precision is within 10^{-14}, and our algorithm in double precision compute the location information up to 14 digits.

To compare the results of the above algorithm, in this subsection, we will formulate the equivalent optimization problem by adding some slack variables. It is well known that Problem (5.1) can be transformed into the following

n	t^*	$\phi(t^*)$
25	0.86729554314871551284	7.9620602967248421084E-2
100	0.89955488860193336250	4.5704003554959619992E-2
400	0.92014479324536438793	2.4522258602174083534E-2
900	0.92779926904699983995	1.6741738132066441762E-2
1600	0.93178840227375636194	1.2707251306191893284E-2
2500	0.93423560762213550127	1.0239138784088078273E-2

(a) Results with multi-precision Fortran (Exflib library).

n	t^*	$\phi(t^*)$	Time
25	0.8672955431487154**8648**	7.9620602967248599313E-2	3.0E-4
100	0.8995548886019333**3345**	4.5704003554959626854E-2	9.2E-3
400	0.9201447932453648**0043**	2.4522258602173718778E-2	0.378
900	0.927799269047000**71866**	1.6741738132065808742E-2	4.34
1600	0.931788402273756**69958**	1.2707251306191658102E-2	24.42
2500	0.93423560762213**675446**	1.0239138784087109535E-2	94.78

(b) Results with double precision Fortran. Bold numbers are different with the results in Table 6.2a

Table 6.2: Numerical solutions of Algorithm 2 to the data set (6.1) using double and multi precisions

nonlinear optimization problem :

$$\begin{aligned} \text{minimize} \quad & f(s,t) = s \\ \text{subject to} \quad & g_j(s,t) = s - \phi_j^2(t) \geq 0, \quad j = 1, \cdots, n \end{aligned} \tag{6.2}$$

where s is a slack variable. The augmented Lagrangian method can be used to solve the above problem and there are well known software packages that use the method.

In order to compare Algorithm 2 with some other optimization techniques, Problem (6.2) was solved by using a general nonlinear programming package ALGENCAN, described in [1] and available in the TANGO web page `http://www.ime.usp.br/~egbirgin/tango/`. Table 6.3 lists various results of ALGENCAN package, together with the values of various stopping criteria

(ε_{feas} and ε_{opt}) and initial guesses. It can be seen from this table that, although the computation time is less than that of our proposed Algorithm 2, the accuracy is considerable less. Moreover, in some cases convergence is not guaranteed within a finite number of iterations. As Table 6.3c shows, the iteration fails to converge to specified tolerance when n is equal to 1600.

6.3 Test case 3

As shown in Section 5.1.2, the computational complexity of our algorithm is $O(n^3)$. This means that it requires 8 times longer computation time for simulating with two times more data.

Table 6.4 shows the averaged computation time of the proposed algorithm. The results of table are obtained by using randomly generated n data points, *i.e.*, $n = 100, 200, 400, \cdots, 6400$, and the values of computation time are averaged over 20 trials. Also the table contains computational complexity which increases in cubic order with the number of data points n. These results confirm that the computational cost behaves like a cubic polynomial in the number of points, as discussed above.

6.4 Conclusions

We have investigated the suggested minimax problem applied to facility location and nano-scale circuit design. Here we also consider the general weighted case. Although finding all elements of $\mathcal{I}$ costs $\mathcal{O}(n^3)$ computational complicity, the computation is simple and easily parallelelizable. Thus the rapid development of computing devices can also improve the efficiency of the algorithm. Also we emphasize that our proposed algorithm is very stable and efficient since it finds a solution in a predicted amount of floating operations as it is

n	t^*	$\phi(t^*)$	Time	It
25	0.86729554316852064399	7.9620602966118322885E-2	0.01	12
100	0.89955494031656146880	4.5704001366303016740E-2	0.01	11
400	0.92014483986480211097	2.4522257562902962518E-2	0.01	13
900	0.92779941103548424496	1.6741604006454677278E-2	0.03	12
1600	0.93178840425354281240	1.2707251283536964009E-2	0.06	13
2500	0.93423560877152289627	1.0239138773443411806E-2	0.09	14

(a) $\varepsilon_{feas} = 10^{-8}$, $\varepsilon_{opt} = 10^{-8}$ and initial point $= (1, 1)$

n	t^*	$\phi(t^*)$	Time	It
25	0.86729554314873358311	7.96206029672474752124E-2	0.01	18
100	0.89955488860189147803	4.57040035549614656607E-2	0.01	16
400	0.92014479324537756799	2.45222586021740483753E-2	0.02	15
900	0.92779926904693910127	1.67417381320111025023E-2	0.07	18
1600	0.93178840227382386807	1.27072513064675936267E-2	0.10	16
2500	0.93423560762211532715	1.02391387840712524276E-2	0.14	16

(b) $\varepsilon_{feas} = 10^{-14}$, $\varepsilon_{opt} = 10^{-14}$ and initial point $= (1, 1)$

n	t^*	$\phi(t^*)$	Time	It
25	0.86729554314871537545	7.96206029672484882909E-2	0.02	25
100	0.89955488860193333344	4.57040035549596268538E-2	0.02	25
400	0.92014479324536524451	2.45222586021736979611E-2	0.04	23
900	0.92779926904700138479	1.67417381320656422083E-2	0.11	28
1600	Not converged until iter = 999999999			
2500	0.93423560762213775365	1.02391387840862751329E-2	0.18	26

(c) $\varepsilon_{feas} = 10^{-16}$, $\varepsilon_{opt} = 10^{-16}$ and initial point $= (1, 1)$

n	t^*	$\phi(t^*)$	Time	It
25	0.86729554314871537545	7.96206029672484882909E-2	0.01	24
100	0.89955488860193344446	4.57040035549596129760E-2	0.03	25
400	0.92014479324536480043	2.45222586021736632667E-2	0.06	25
900	0.92779926904700327217	1.67417381320656977195E-2	0.11	30
1600	0.93178840227375581140	1.27072513061914308535E-2	0.12	21
2500	0.93423560762213797570	1.02391387840862716635E-2	0.24	30

(d) $\varepsilon_{feas} = 10^{-16}$, $\varepsilon_{opt} = 10^{-16}$ and initial point $= (0.5, 2)$

Table 6.3: Numerical solutions of Problem (6.2) by ALGENCAN to the data set (6.1), together with the values of various stopping criteria and initial guess.

Number of data(n)	Time	order
100	1.175E-2	-
200	8.992E-2	7.65
400	0.6912	7.69
800	5.4541	7.89
1600	43.203	7.92
3200	343.98	7.96

Table 6.4: Comparison of averaged computation time for the proposed algorithm

based on an exact search procedure. In this thesis, we simulated an optimization problem with weighted distance functions, but in the case of equi-weighted distance functions the algorithm has halved computing cost.

A further research about reducing the number of possible optimal points will be done, which will improve the presented algorithm significantly.

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국문초록

본 논문에서는 두 가지 주제의 최적화 문제에 대한 해석적 분석과 수치적 검증에 대한 내용을 논하였다. 첫 번째 장에서는 데이터 정보로부터 주어진 상미분 방정식의 매개변수 함수를 추정하는 방법을 다루었는데, 특별히 선형 일차 상미분 방정식을 가정하였다. 또한 매개변수 함수의 경우에는 조각적으로 정의된 상수 함수를 가정하였는데, 이를 통해 시간에 따라 변화하는 매개변수의 물리적인 특성을 반영하도록 하였다. 이 때 매개변수 함수의 불연속이 발생하는 점에 대해서는 그 개수와 위치에 대한 정보를 모두 미지수라고 가정하였으며, 총변량을 죄소화하도록 제안된 알고리즘을 통해 매개변수 함수를 계산하였다. 이를 통해 데이터를 모두 지나도록 하는 상미분 방정식의 최적화된 매개변수 함수를 구하도록 하였다.

두 번째 장에서는 인쇄 배선 회로 기판의 최적화된 배치 및 배선에 대한 내용을 다루었다. 주어진 두 개의 고정된 점을 지나는 원의 원주와 주어진 데이터 사이의 최대 길이를 최소화하는 최적화 문제를 가정하였다. 최적화된 해를 찾기 위한 해석적으로 정확한 알고리즘이 고안되었으며, 이에 대해 수치적 분석이 수행되었다. 이 때 제안된 알고리즘의 분석을 위해 배수 정도 계산을 통해 주어진 알고리즘의 정확도에 대한 분석을 하였으며, 다른 최적화 소프트웨어와의 비교를 통해 계산 속도와 정밀성에 대해 논하였다. 또한 계산 복잡도 이론에 대한 분석과 수치적 검증도 수행하였다.

주요어: 최적화, 매개변수 추정, 최대 최소 문제,

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